



PDBj
Protein Data Bank Japan

PDBjの最近の活動とwwPDB の活動方針

大阪大学蛋白質研究所
栗栖源嗣

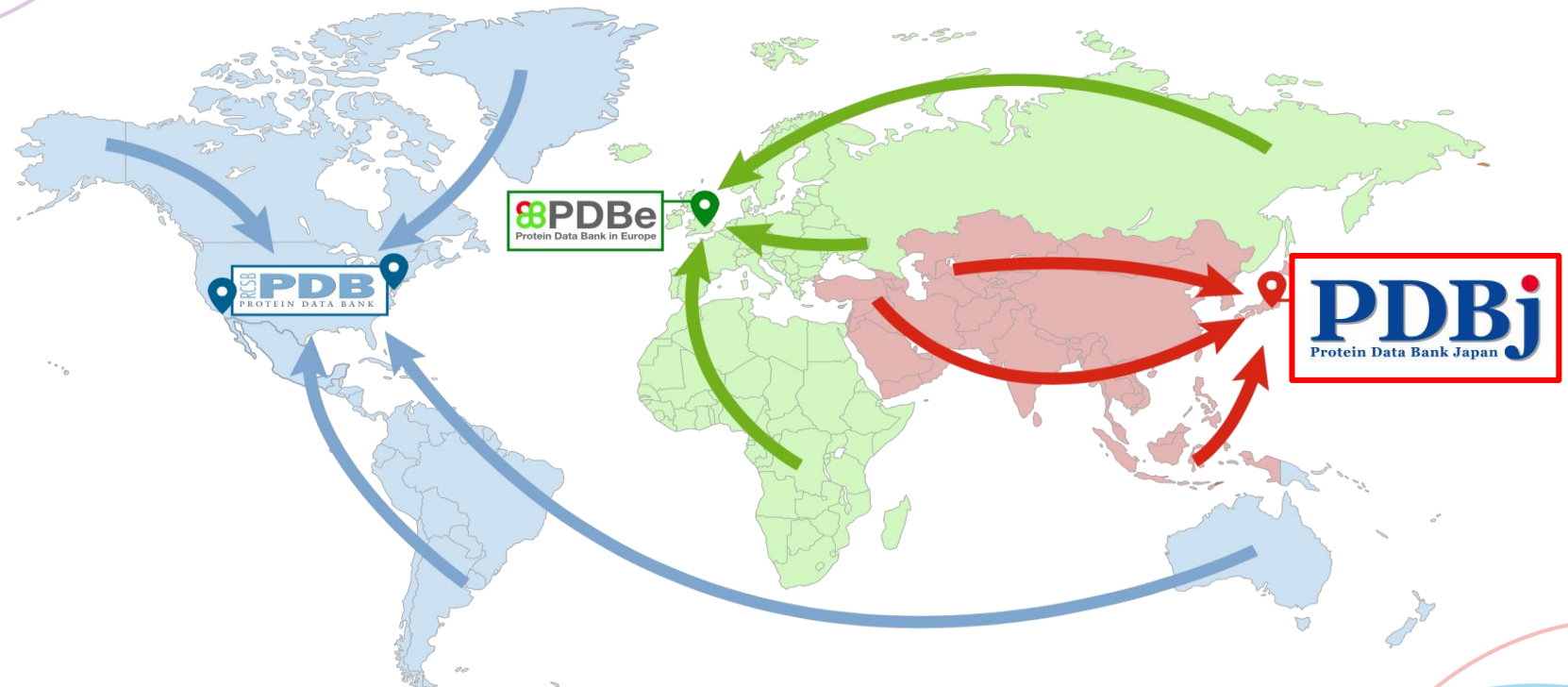
PDBj は **wwPDB** と **JBIportal** のメンバーです。
Protein Data Bank Japan WORLDWIDE PROTEIN DATA BANK Japan alliance for Bioscience Information



Protein Data Bank Japan :



アジアの蛋白質構造データセンターです



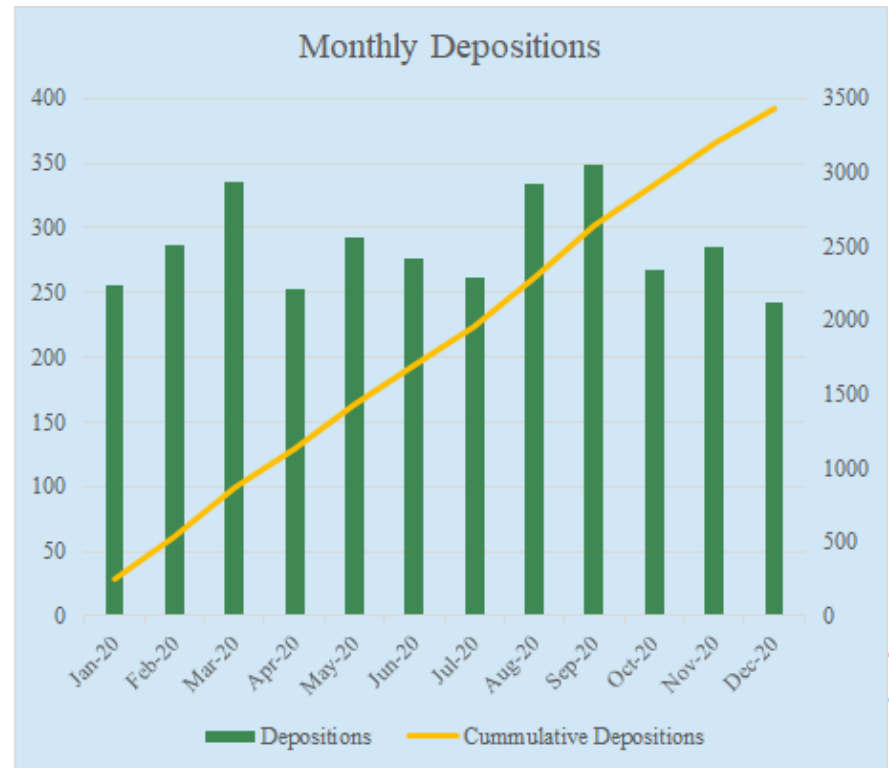
登録は国際分業で、管理は国際共同で、利用提供は独立に行っています。





PDBjで処理したエントリー数

	X-ray	NMR	EM *1)	Others	Depositions	Cumulative Depositions
Jan-20	210	5	40		255	255
Feb-20	233	10	43		286	541
Mar-20	247	24	65		336	877
Apr-20	181	14	57	1	253	1130
May-20	258	3	30	2	293	1423
Jun-20	227	4	45		276	1699
Jul-20	205	8	48		261	1960
Aug-20	267	10	57		334	2294
Sep-20	242	14	92	1	349	2643
Oct-20	207	4	55	1	267	2910
Nov-20	231	8	45	1	285	3195
Dec-20	182	5	56		243	3438
Total	2690	109	633	6	3438	

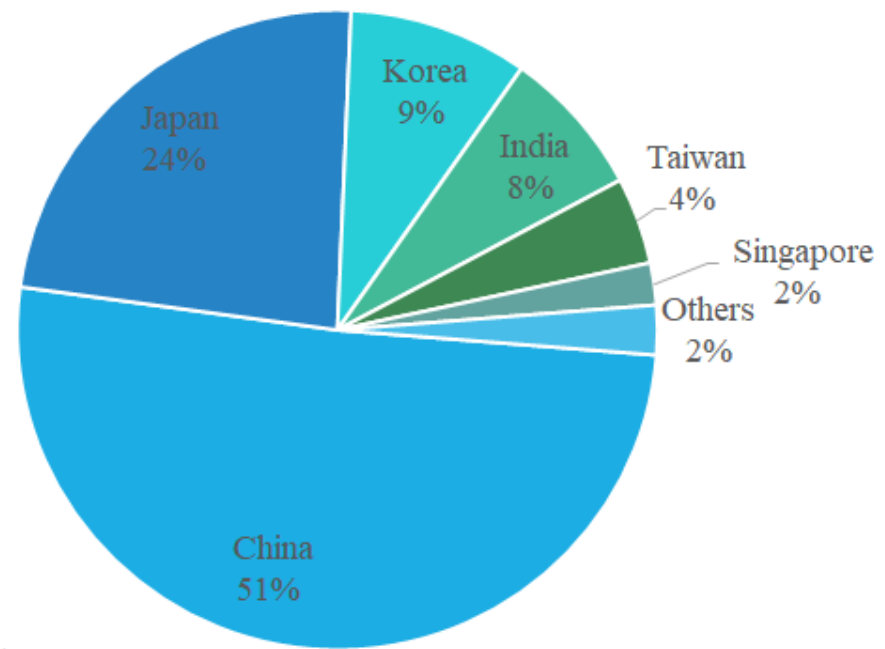


*1) excluding map only entries



PDBjで処理したPDBエントリーの 国・地域別割合

Country/Region *2)	Depositions
China	1750
Japan	809
Korea	312
India	257
Taiwan	151
Singapore	73
Thailand	41
Hong Kong	34
Malaysia	5
Saudi Arabia	3
Turkey	2
Macao	1



*2) Country/Region a depositor selected on creating a session



wwPDBのメンバーが3つのデータベースを共同で管理運営

- PDB

- XYZの原始座標
- X線解析の構造因子

- BMRB

- 化学シフト
- 距離/角度制限情報
- その他

- EMDB

- マップ



WORLDWIDE
PDB
PROTEIN DATA BANK

CORE
ARCHIVES

PDB
BMRB
EMDB

CORE
MEMBERS

RCSB PDB
PDBe, PDBj,
BMRB, EMDB



PDBへの登録を論文等に掲載される際 のお願い

PDBエントリーは、wwPDBのメンバーが国際分業で処理します。登録について論文中に記載される場合は、以下の例のようにお願いします。

例1 *“The coordinates and structure factors for the structures reported here are deposited to the worldwide Protein Data Bank and available from the Protein Data Bank Japan with accession codes of #####.”*

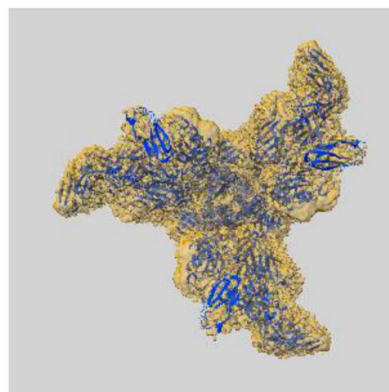
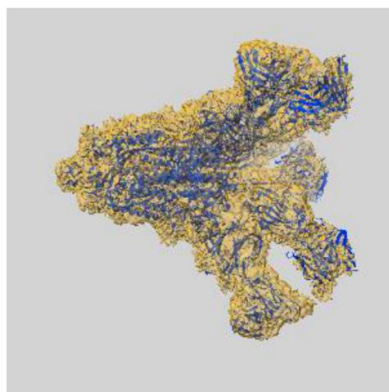
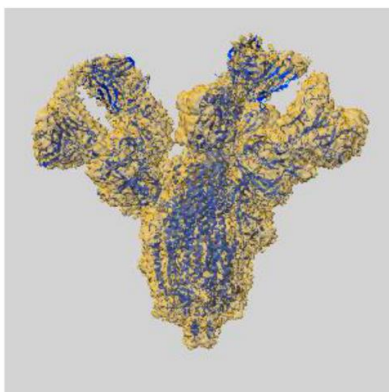
例2 *“The cryo-EM density map is deposited in the Electron Microscopy Data Bank under accession number EMD-#####. The atomic models of the cryo-EM structures are deposited in the worldwide Protein Data Bank (wwPDB) under accession numbers ##### and #####, respectively”*

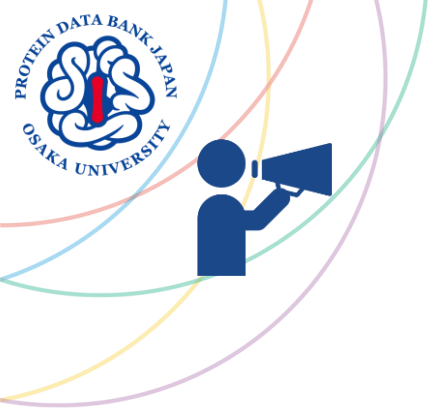
例3 *“The coordinates for YOUR PROTEIN1 and YOUR PROTEIN2 are available as PDB entries ##### and #####, respectively. The resonance assignment for YOUR PROTEIN 1 has been deposited in the Biological Magnetic Resonance Bank as accession number #####.”*



新しいEM検証レポート

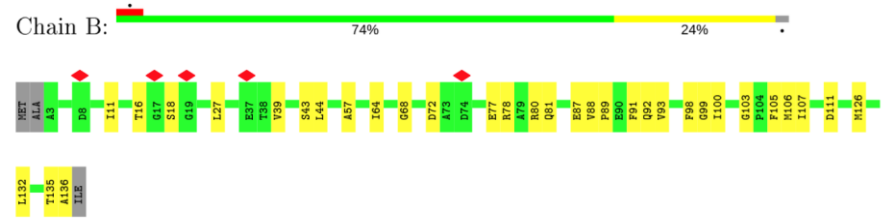
- 2021年1月12日からEM構造とEMマップの検証レポートが新しくなりました！
- 詳細は以下のウェブをご覧ください
www.pdb.org/validation/2017/EMValidationReportHelp



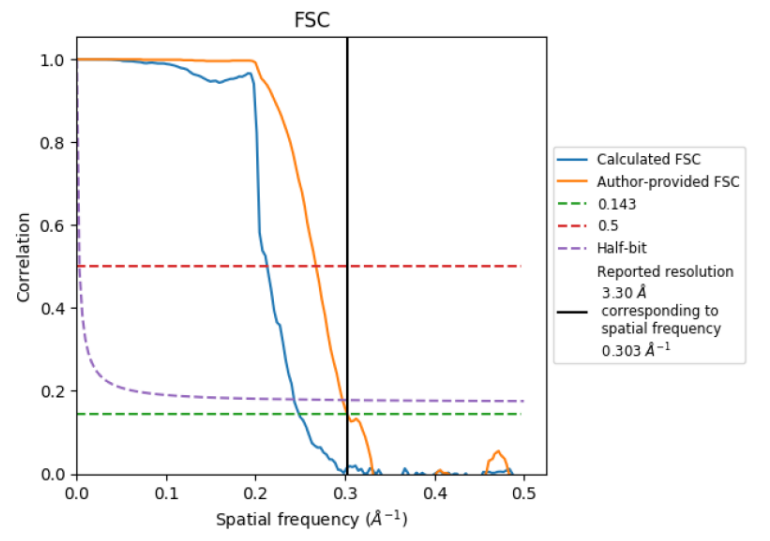
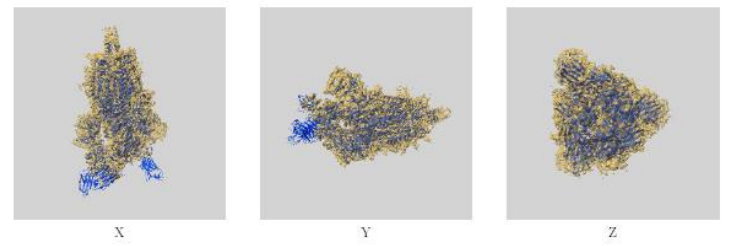


新しいEM検証レポート

• Molecule 1: Tail tube protein Rcc01691



- Map + model quality
- Map-model fit
 - Per-residue quality plots
 - Image of map + model overlaid
- Improvements to Fourier-Shell Correlation (FSC) plot:
 - Limited cut-offs to '0.143', '0.5' and 'halfbit' unless another criteria used
 - FSC curves provided by the authors and recalculated from the deposited half-maps shown in one plot





新しいEM検証レポート

- 専門家に集まっていたいただいて，EM検証の方針を継続的に審議しています。





(古い)PDBフォーマットの限界

Field No.	Column range	FORTTRAN format	Description
1.	1 - 6	A6	Record ID (eg ATOM, HETATM)
2.	7 - 11	I5	Atom serial number
-	12 - 12	1X	Blank
3.	13 - 16	A4	Atom name (eg " CA " , " ND1")
4.	17 - 17	A1	Alternative location code (if any)
5.	18 - 20	A3	Standard 3-letter amino acid code for residue
-	21 - 21	1X	Blank
6.	22 - 22	A1	Chain identifier code
7.	23 - 26	I4	Residue sequence number
8.	27 - 27	A1	Insertion code (if any)
-	28 - 30	3X	Blank
9.	31 - 38	F8.3	Atom's x-coordinate
10.	39 - 46	F8.3	Atom's y-coordinate
11.	47 - 54	F8.3	Atom's z-coordinate
12.	55 - 60	F6.2	Occupancy value for atom
13.	61 - 66	F6.2	B-value (thermal factor)
-	67 - 67	1X	Blank
14.	68 - 70	I3	Footnote number

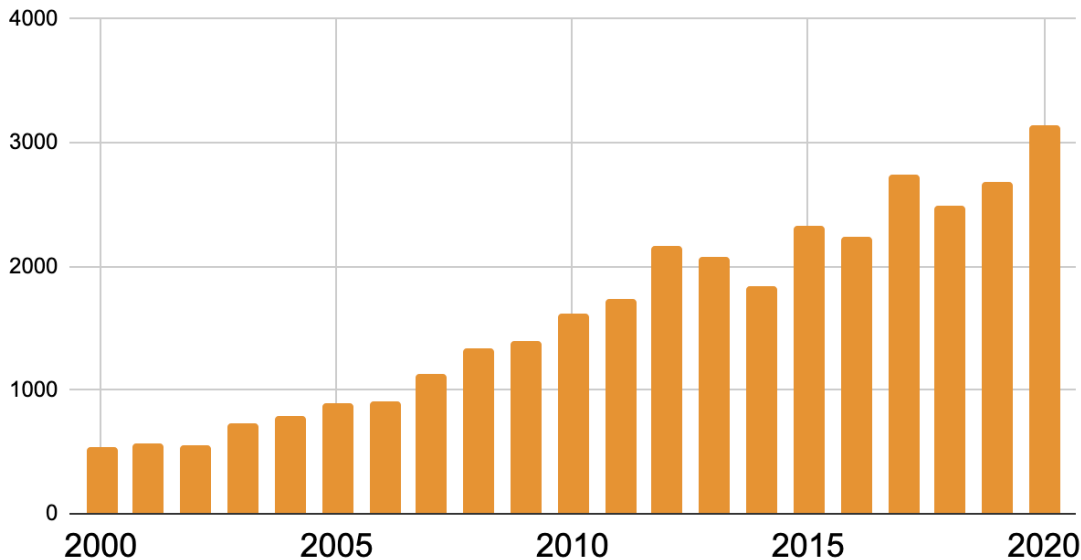
1	2	3	4	5	6
12345678901234567890123456789012345678901234567890123456789012345678					
ATOM	1751	N	GLY C 250	32.286	1.882 43.206 1.00 22.00
ATOM	1752	CA	GLY C 250	32.365	1.086 41.969 1.00 21.39
ATOM	1753	C	GLY C 250	31.538	1.735 40.864 1.00 20.79
ATOM	1754	O	GLY C 250	30.621	2.527 41.152 1.00 21.58



化合物IDが4桁になる

- PDBフォーマットでつかう3文字の化合物IDが2年程度で足りなくなります
- 以降の新規データはPDBx/mmCIFでのみ提供されます

Number of New Chemical Component Entries Created Each Year





PDB IDは8桁になる

- 4文字のPDB IDも近い将来枯渇します
- 既に8文字のPDB IDでデータが提供されています
- wwpdb.org/pdb?id=pdb_00006lu7



WORLDWIDE PDB PROTEIN DATA BANK

PDB Entry - 6LU7 (Status - Released)

Summary information:

Title: The crystal structure of COVID-19 main protease in complex with an inhibitor N3

DOI: [10.2210/pdb6lu7/pdb](https://doi.org/10.2210/pdb6lu7/pdb)

Primary publication DOI: [10.1038/s41586-020-2223-y](https://doi.org/10.1038/s41586-020-2223-y)

Entry authors: Liu, X., Zhang, B., Jin, Z., Yang, H., Rao, Z.

Initial deposition on: 26 January 2020

Initial release on: 5 February 2020

Latest revision on: 10 March 2021

Downloads:

- Structure coordinates (PDBx/mmCIF)
- Structure coordinates (PDBML)
- Structure coordinates (PDB)
- X-ray diffraction data (PDBx/mmCIF)
- Validation report (PDF)
- Validation report (XML)

Links to more resources for 6LU7 at:



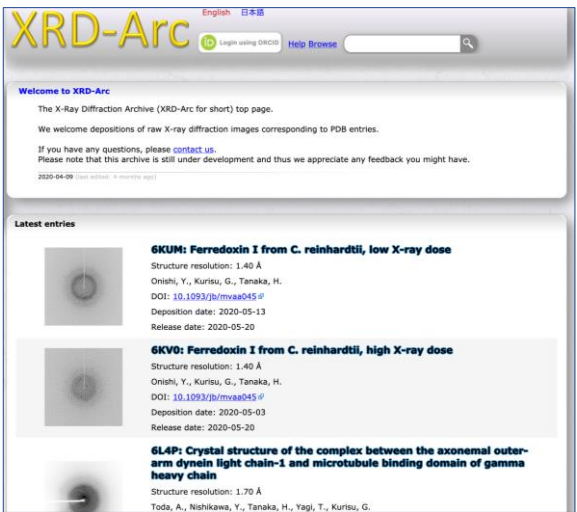
Raw Dataの登録が強く奨励されます

NEW

<https://xrda.pdbj.org>

<https://empiar.pdbj.org>

<https://deposit-bmrdb.pdbj.org>



XRD-Arc English 日本語

Welcome to XRD-Arc

The X-Ray Diffraction Archive (XRD-Arc for short) top page.

We welcome depositions of raw X-ray diffraction images corresponding to PDB entries.

If you have any questions, please [contact us](#).

Please note that this archive is still under development and thus we appreciate any feedback you might have.

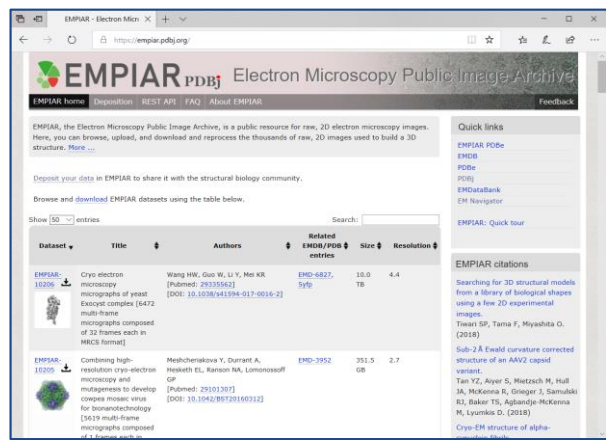
2020-04-09 (last edited: 7 months ago)

Latest entries

6KUM: Ferredoxin I from *C. reinhardtii*, low X-ray dose
Structure resolution: 1.40 Å
Onishi, Y., Kurisu, G., Tanaka, H.
DOI: [10.1093/jb/mxaa045](https://doi.org/10.1093/jb/mxaa045)
Deposition date: 2020-05-13
Release date: 2020-05-20

6KV0: Ferredoxin I from *C. reinhardtii*, high X-ray dose
Structure resolution: 1.40 Å
Onishi, Y., Kurisu, G., Tanaka, H.
DOI: [10.1093/jb/mxaa045](https://doi.org/10.1093/jb/mxaa045)
Deposition date: 2020-05-03
Release date: 2020-05-20

6L4P: Crystal structure of the complex between the axonemal outer-arm dynein light chain-1 and microtubule binding domain of gamma heavy chain
Structure resolution: 1.70 Å
Toda, A., Nishikawa, Y., Tanaka, H., Yagi, T., Kurisu, G.



EMPIAR PDB Electron Microscopy Public Image Archive

EMPIAR, the Electron Microscopy Public Image Archive, is a public resource for raw, 2D electron microscopy images. Here, you can browse, upload, and download and reprocess the thousands of raw, 2D images used to build a 3D structure. [More ...](#)

Deposit your data in EMPIAR to share it with the structural biology community.

Browse and download EMPIAR datasets using the table below.

Show [50] entries

Dataset	Title	Authors	Related EMDB/PDB entries	Size	Resolution
EMPIAR-10206	Cryo electron microscopy micrographs of yeast <i>Esocet</i> complex (6472 multi-frame micrographs composed of 32 frames each in MRCS format)	Wang HW, Guo W, Li Y, Mei KR [PubMed: 2933562] DOI: 10.1038/s41594-017-0016-2	EMD-6837, 5yfp, TB	10.0	4.4
EMPIAR-10205	Combining high-resolution cryo-electron microscopy and mutagenesis to develop chaperone rescue virus for biomanufacturing [2019 multi-frame micrographs composed of 2.1 frames each in MRCS format]	Mecherikavala Y, Durant A, Heppelth KL, Karpov M, Lemmoniauff GP [PubMed: 3101370] DOI: 10.1038/s41594-017-0016-2	EMD-5952	351.5	2.7

EMPIAR citations

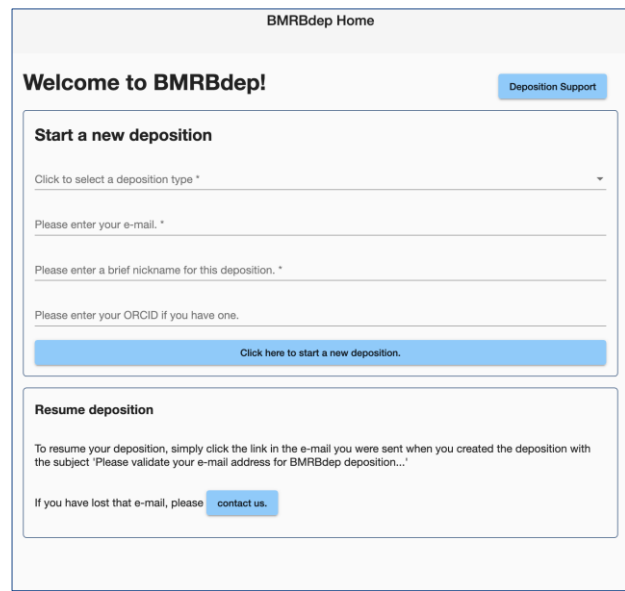
Searching for 3D structural models from a library of biological shapes using a few 2D experimental images.

Tsutsui SP, Tama F, Miyashita O. (2018)

Sub-2 Å Ewald curvature corrected structure of an AA2' capid variant.

Tan YZ, Ayer S, Mietzsch M, Hill JA, McKenna B, Grainger J, Samulski RJ, Baker TS, Agbandje-McKenna M, Lyumkis D. (2018)

Cryo-EM structure of alpha-



BMRBdep Home

Welcome to BMRBdep! [Deposition Support](#)

Start a new deposition

Click to select a deposition type *

Please enter your e-mail. *

Please enter a brief nickname for this deposition. *

Please enter your ORCID if you have one.

[Click here to start a new deposition.](#)

Resume deposition

To resume your deposition, simply click the link in the e-mail you were sent when you created the deposition with the subject 'Please validate your e-mail address for BMRBdep deposition...'

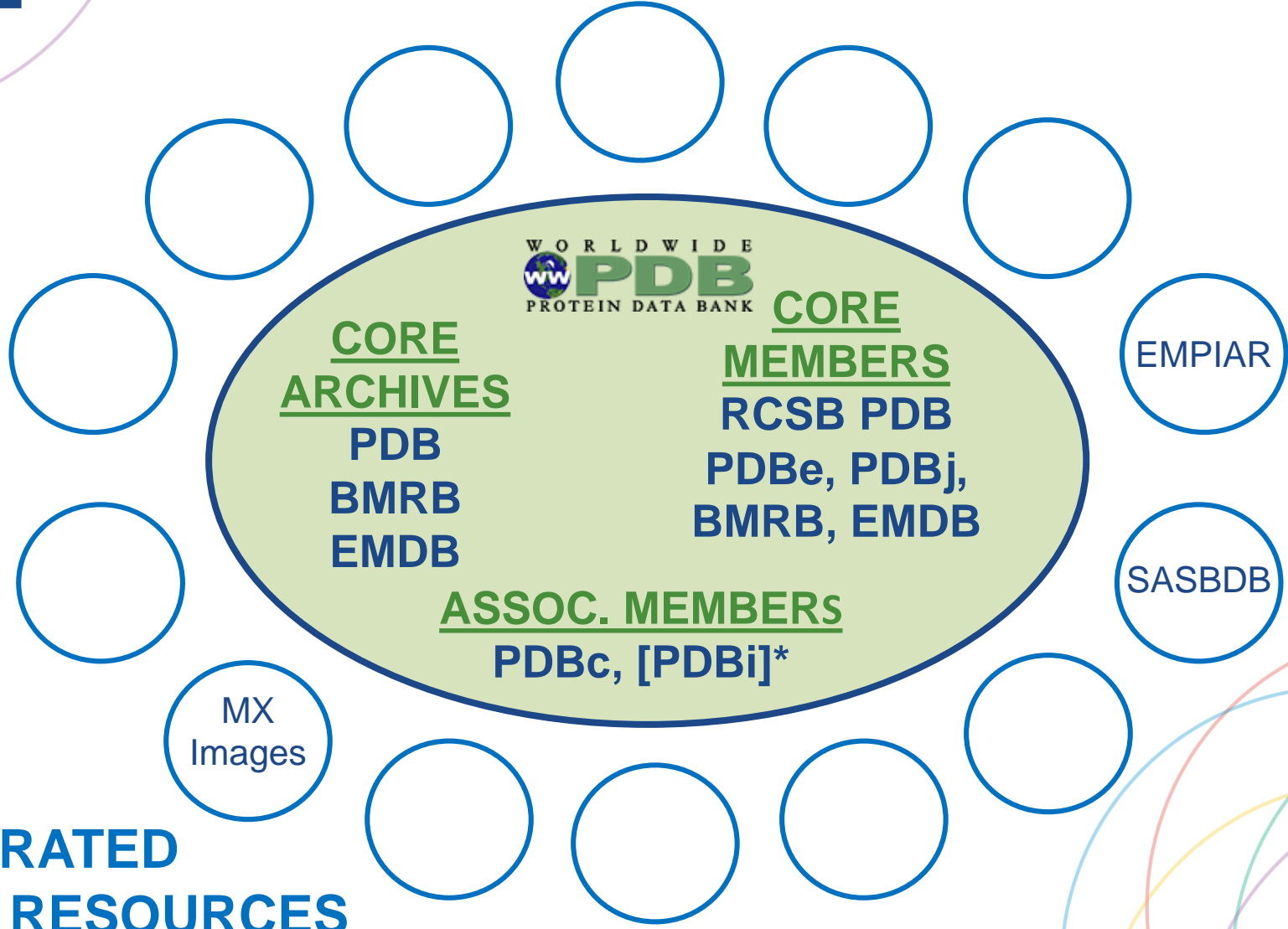
If you have lost that e-mail, please [contact us](#).



All three experimental data types are archived in Asia!



PDBcとPDBiが誕生します



**FEDERATED
DATA RESOURCES**



PDB50周年記念シンポ

- PDBは1971年に誕生し、今年で50歳
- 50周年記念シンポジウムを日本生物物理学会のサテライトとして11月24日にオンライン開催します

ぜひご参加ください

**PROTEIN
DATA BANK**



Acknowledgements

